Lee-Yang zeros and phase transitions in nonequilibrium steady states

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We consider how the Lee-Yang description of phase transitions in terms of partition function zeros applies to nonequilibrium systems. Here one does not have a partition function, instead we consider the zeros of a steady-state normalization factor in the complex plane of the transition rates. We obtain the exact distribution of zeros in the thermodynamic limit for a specific model, the boundary-driven asymmetric simple exclusion process. We show that the distributions of zeros at the first and second order nonequilibrium phase transitions of this model follow the patterns known in the Lee-Yang equilibrium theory.

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With equilibrium statistical physics now firmly established as a successful general theory for predicting the macroscopic behavior of many-body systems, attention has more recently turned to the the wider class of nonequilibrium systems. Examples of nonequilibrium systems are those relaxing to thermal equilibrium or those driven into a steady state, far from thermal equilibrium. A general framework for understanding these systems is proving elusive. However, over the last two decades the detailed study of specific models has revealed the wide range of phenomena that may emerge.

It is by now well known that models of driven diffusive systems can exhibit phase transitions in their nonequilibrium steady states [1]. Typically such models comprise one or more species of particles being driven by an external field along with prescribed interactions between the boundaries and the outside world. Applications of these models are diverse and include the kinetics of biopolymerization [2], transport across a membrane [3] and traffic flow [4]. From a more fundamental viewpoint, the interest lies in the richness of collective phenomena displayed, including jamming [5] and spontaneous symmetry breaking [6], even in one dimension.

Half a century ago Lee and Yang provided a theory of equilibrium phase transitions based around the zeros of the partition function. In this work we focus on nonequilibrium steady states and how the phase transitions they admit may be placed in the context of the Lee-Yang theory. In the original exposition [7] the fugacity of a gas was generalized to the complex plane and the zeros of the grand-canonical partition function in this plane were considered. In particular, it was shown that the free energy is analytic in any region of the complex-fugacity plane devoid of any zeros. Conversely, there are nonanalyticities at points where the density of partition function zeros accumulate in the thermodynamic limit. These accumulation points correspond to physically observable phase transitions if they lie on the positive real axis. A similar phenomenon occurs in the complex plane of other intensive fugacity-like variables. For example, Lee and Yang also showed [8] that the zeros of the Ising model partition in the complex plane of activity (defined as $\exp(-h/T)$ where h is magnetic field and T temperature) lie on the unit circle. Similarly, partition function zeros in the complex temperature plane also accumulate at phase transition points [9, 10]. The applicability of the Lee-Yang theory to equilibrium transitions driven by intensive field-like variables can be understood from the fact that, mathematically, these variables play similar roles in the partition function.

The difficulty in applying the Lee-Yang theory to, e.g., the steady state of a driven diffusive system is that one does not have to hand a partition function defined in terms of thermodynamic state variables. However, one can always define a quantity Z as a sum of the steady state weights (unnormalized probabilities) $f(\mathcal{C})$:

$$Z = \sum_{\mathcal{C}} f(\mathcal{C}) \ . \tag{1}$$

Thus the probability of a configuration is given by $P(\mathcal{C}) = f(\mathcal{C})/Z$. In this work, we treat the normalization Z as a nonequilibrium analog of the partition function.

In order to obtain Z one still has to calculate the steady state weights. Up to a multiplicative factor they are implied by the transition rates $W(\mathcal{C} \to \mathcal{C}')$ that define the model through the requirement that the total inflow of probability into a given configuration $\mathcal{C}$ must be balanced by the outflow, i.e.,

$$\sum_{\mathcal{C}' \neq \mathcal{C}} [f(\mathcal{C}')W(\mathcal{C}' \to \mathcal{C}) - f(\mathcal{C})W(\mathcal{C} \to \mathcal{C}')] = 0 \ . \tag{2}$$

The solution of this set of equations for the steady-state weights $f(\mathcal{C})$ can, in principle, be obtained using standard methods, such as Gaussian elimination, Cramer's rule or graphically [11]. If one applies such a method, the weights can always be written as polynomials of the elementary transition rates. Thus, for a finite system, Z is also a polynomial of the transition rates.

In this work we generalize the transition rates to the complex plane and in doing so consider the zeros of the

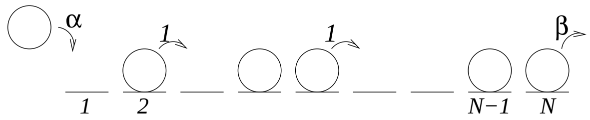

FIG. 1: Dynamics of the ASEP. The arrow labels indicate the rates at which the corresponding transitions occur; site labels are also indicated.

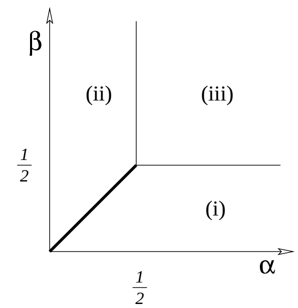

FIG. 2: Phase diagram of the ASEP.

partition function. In analogy with the Lee-Yang picture for equilibrium systems, for a phase transition to arise we expect the zeros to pinch the real axis at a point which corresponds to a (real) critical transition rate.

As an aside, we note that the general methods of solving (2) mentioned above are rarely tractable when the number of configurations becomes large. One exception is when the system satisfies detailed balance. In this case, each term within the square brackets in (2) is identically zero and it is easy to construct the set of steady-state weights as Boltzmann weights with respect to an energy function. The resulting Z is then an equilibrium partition function. A simple example of such a system is the Ising model evolving under Glauber dynamics wherein studying the zeros of the partition function as a function of the transition rate would be equivalent to studying the complex-temperature zeros.

In the present work, however, we are interested in models which do not satisfy detailed balance and hence for which the normalization Z is not *a priori* known. This makes it difficult to make general statements about the significance of the normalization Z. We have argued that a nonequilibrium phase transition will be signaled by an accumulation of the zeros of Z in the complex plane of transition rates towards the real axis. We demonstrate this in the case of a particular nonequilibrium model for which an expression for Z is exactly known and we can calcuate the distribution of zeros analytically. We find that these zeros lie on circles in the complex plane of an appropriately chosen function of a transition rate that plays the role of a fugacity. The characteristic properties of the distributions of partition function zeros at first and second order equilibrium transitions [7, 10, 12] are also exhibited in this nonequilibrium case. In short, we show how the the Lee-Yang theory of phase transitions generalizes to a nonequilibrium steady state.

Before discussing the model and our results in greater detail, we wish to remark how our study differs from a related work due to Arndt [13]. The aim of that investigation was to locate a phase transition induced by varying the relative numbers of different particle species in a particle-conserving driven diffusive system. To this end, a fugacity-like quantity was introduced in an *ad hoc* way. Physically, this corresponds to placing the driven diffusive system in contact with a particle reservoir thus introducing equilibrium fluctuations in the particle densities. We stress that in the present work, it is elementary transition rates, which need not have any connection to intensive field (fugacity-like) variables, that are generalized to the complex plane.

We now introduce the model we consider, namely the one-dimensional asymmetric simple exclusion process (ASEP) with open boundaries. Since its introduction [2, 14] this model has received a great deal of attention—see, e.g., [11, 15] for further details and references. The model comprises a lattice of N sites, each of which may be occupied or empty. In an infinitesimal time interval $\mathrm{d}t$ one of the following transitions may occur: a particle may hop one site to the right with probability $\mathrm{d}t$ (i.e. at unit rate) subject to the receiving site being vacant; a particle may be inserted onto the leftmost site (if vacant) with probability $\alpha \mathrm{d}t$ or a particle occupying the rightmost site (if present) may be removed with probability $\beta \mathrm{d}t$. Fig. 1 illustrates the microscopic dynamics.

As outlined above, there is a current (defined as the flux of particles between neighbouring sites per unit time) in the steady state which in the thermodynamic limit $N \to \infty$ exhibits nonanalyticities as the boundary rates α and β are varied. These are associated with phase transitions, and the phase diagram is given in Fig. 2.

Phase (i) is a high-density phase with a density profile that decays exponentially towards the right boundary. In this phase the current $J = \beta(1-\beta)$. Since the ASEP is invariant under particle-hole exchange and the swap $\alpha \leftrightarrow \beta$, it follows that phase (ii) is a low-density phase that has an exponential decay in the density profile from the left boundary and a current $J = \alpha(1-\alpha)$. At the first order transition line $\alpha = \beta < \frac{1}{2}$ the current exhibits a discontinuity in its first derivative. Here the system exhibits a shock front separating regions of high and low density; this is an example of phase coexistence at a nonequilibrium phase transition.

In phase (iii), the current assumes a constant value $J = \frac{1}{4}$ which is the largest possible current admitted for any combination of α and β. Hence phase (iii) is called the maximal current phase. This phase has the interesting feature that the density profile decays as a power-law from both boundaries and hence at the transition from either phase (i) or (ii) to phase (iii) a correlation length diverges. Additionally, J has a discontinuity in its second

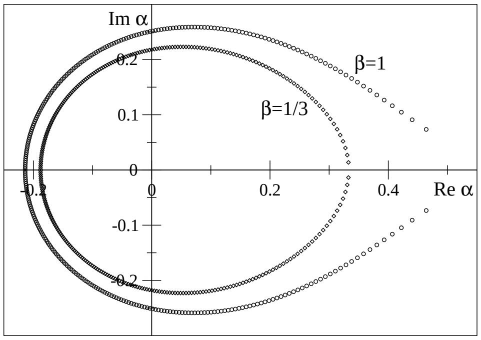

FIG. 3: Zeros of the normalization (3) in the complex-α plane for $\beta = \frac{1}{3}, 1$. In both cases the lattice size N is 300.

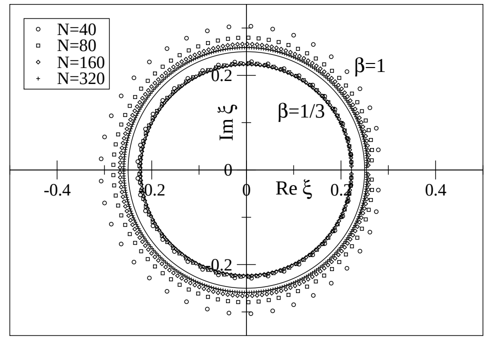

FIG. 4: Zeros of the normalization (3) in the complex-$\xi = \alpha(1-\alpha)$ plane for $\beta = \frac{1}{3}, 1$ and $N = 80, 160, 320$.

derivative and so this is a second-order transition.

These results are known mainly from the exact solution [16, 17]. The two key results we call upon here are that the normalization for an N-site system Z_N is given by

$$Z_N = \sum_{p=1}^{N} \frac{p(2N-1-p)!}{N!(N-p)!} \frac{(1/\beta)^{p+1} - (1/\alpha)^{p+1}}{(1/\beta) - (1/\alpha)} \qquad (3)$$

and the current by $J = Z_{N-1}/Z_N$. In order later to construct the distribution of the zeros of Z_N for the ASEP we also need the large-N forms of Z_N. From the exact solution it can be shown that for all α, β, $Z_N \sim AJ^{-N}N^{\gamma}$ where J is the current and A, γ depend only on the phase being considered. We see $\ln J$ is the extensive part of $-\ln Z_N$ and thus $\ln J$ plays the role of the free energy and J the fugacity for this nonequilibrium system.

We now consider the zeros of Z_N given by (3) in the complex-α plane at fixed β [18]. (The symmetry in α and β of Z_N implies that one would obtain the same pattern of zeros in the complex-β plane at fixed α). Using Mathematica, we obtained numerical estimates of the zeros of Z_N for system size (and number of zeros) $N = 300$ and $\beta = 1, \frac{1}{3}$. The results are shown in Fig. 3.

For the case $\beta = \frac{1}{3}$, the zeros appear to approach the positive real α axis at a value $\alpha_c = \frac{1}{3}$, coincident with the first-order phase transition point in this regime. The plot for the case $\beta = 1$ is suggestive of a slow accumulation of the zeros to the positive real α axis at $\alpha_c = \frac{1}{2}$, i.e. the second-order phase transition point. It appears also in this case that the zeros approach the real axis at an angle $\frac{\pi}{4}$ as opposed to an angle $\frac{\pi}{2}$ at the first-order transition. We will shortly demonstrate that the above assertions—consistent with the patterns of zeros at first- and second-order phase transitions known from the equilibrium Lee-Yang theory [7, 10, 12]—are correct.

It is useful to make a change of variable from α to $\xi = \alpha(1-\alpha)$ (note that in the low density phase $\xi = J$) and we plot the numerically-obtained zeros in the complex-ξ plane in Fig. 4. For both $\beta = 1, \frac{1}{3}$, it appears that, as $N \to \infty$, the zeros become uniformly distributed around a circle of radius $\xi_c = \alpha_c(1-\alpha_c)$ (these circles are shown as solid lines in the figure). We shall now show how to obtain this result analytically.

We first note (for a proof see [19]) that for any polynomial $p_N(\xi)$ with N zeros, its density of zeros $\rho(x,y)$ in the complex $\xi = x + iy$ plane is given by $\rho(x,y) = 2\pi\nabla^2 \ln|p_N(\xi)|$ where $\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$. In the thermodynamic limit ($N \to \infty$) we expect a continuous distribution of zeros and wish to normalize ρ so that its integral over all space is unity. We thus define the key quantity

$$\phi = \lim_{N\to\infty} \frac{\ln|Z_N|}{N} \qquad (4)$$

so that $\rho = 2\pi\nabla^2\phi$. In equilibrium statistical physics ϕ would be interpreted as the extensive part of the free energy; as noted above $\phi = -\ln|J|$ for the ASEP.

It is useful to regard ϕ as an 'electrostatic' potential in a two-dimensional space. We introduce the field $\vec{E} = \nabla\phi$ and consider the discontinuities that arise as a line of charge (zeros) is crossed. The appropriate forms of Gauss's and Ampere's laws imply that the component of $\vec{E}$ parallel to a line of zeros separating two phases must be continuous across it whereas the perpendicular component differs by a value $2\pi g(x,y)$ where $g(x,y)$ is the line density of charge (zeros) along the boundary.

The current itself has only two analytic forms. In the interior region of Fig. 4 (i.e., the region that includes $\xi = 0$) $J = \alpha(1-\alpha) = \xi$ and hence $\phi = -\ln|\xi|$. Over the exterior region, the current is constant: $J = \alpha_c(1-\alpha_c) = \xi_c$ and so $\phi = -\ln|\xi_c|$.

The field that results from the potential ϕ is zero in the exterior region and directed radially towards the origin in the interior region; specifically $\vec{E} = -\vec{r}/r^2$ where $\vec{r} = (\mathrm{Re}\,\xi, \mathrm{Im}\,\xi)$. Now, since the component of the electric field parallel to the boundary between the two phases varies continuously and is zero in the exterior region, the phase boundary must lie perpendicular to the field lines in the interior region. In other words, the phase boundary is an equipotential $\phi = -\ln|\xi| = \text{const} \Longrightarrow |\xi| = \xi_c$ since the boundary must pass through the transition point at $\xi = \xi_c$. The line-density of zeros $g(\theta)$ along the circle $\xi =$

$\xi_c e^{i\theta}$ can be calculated by noting that the perpendicular component of the field at the boundary has a magnitude $1/|\xi_c|$. The relationship given above then implies $g(\theta) = (2\pi\xi_c)^{-1}$, i.e., a constant as claimed.

We now use this result to investigate the distribution of zeros near the transition point in the complex-α plane. In the ξ plane, the circle of zeros passes along the line $\mathrm{Re}\,\xi = \xi_c$ which maps onto a curve in the complex $\alpha = u + iv$ plane that has $(u - \frac{1}{2})^2 - v^2 = \frac{1}{4} - \xi_c$. The solution of this equation that describes a line passing through the transition point $\alpha = \alpha_c$ is $u = \frac{1}{2} - (v^2 + \frac{1}{4} - \xi_c)^{1/2}$.

When the phase transition is first order, $\beta < \frac{1}{2}$ and $\xi_c = \beta(1-\beta) < \frac{1}{4}$. Then, the curve of zeros passes smoothly through the transition point $\alpha = \beta$. One can show that the line density of zeros at this point in the complex-α plane is $(1-2\beta)/[2\pi\beta(1-\beta)]$, i.e., nonzero. The fact that the density of zeros is nonzero on the real axis at a first-order phase transition is well-known in the equilibrium Lee-Yang theory [7].

At the second order phase transition ($\beta \geq \frac{1}{2}$ and $\xi_c = \frac{1}{4}$) the line of zeros is given by $u = \frac{1}{2} - |v|$. This means the zeros approach the transition point $\alpha = 1/2$ at an angle of $\frac{\pi}{4}$ to the real axis, meeting at a right angle. If one defines ℓ as the displacement along the straight line of zeros from the transition point, one finds that it varies with $y = \mathrm{Im}\,\xi$ as $\ell = \sqrt{y}$. This implies that the density of zeros behaves as $g(\ell) = \frac{2}{\pi}\frac{\mathrm{d}y}{\mathrm{d}\ell} = \frac{4\ell}{\pi}$. In the equilibrium theory, it is well known that the density of zeros vanishes as a power-law towards the transition point on the real line (see, e.g., [12]), a result we have recovered in this nonequilibrium case.

To summarize, we have shown that the zeros for the normalization of the ASEP accumulate at the phase transition points in the complex plane of transition rates. As in the case of the Lee-Yang theory, a first-order transition is manifested by a nonzero density of zeros at the accumulation point, whereas the density of zeros decays as a power-law towards a continuous transition point.

A point that we have so far ignored is that the normalization (1) is only defined up to a multiplicative factor that depends on the method used to solve Eqn. (2). This additional factor is analogous to that which would appear in an equilibrium partition function after a uniform shift of the energy scale. Although this factor could itself be a polynomial of the transition rates and so introduce additional zeros, one would not expect these spurious zeros to be physically relevant to the phase behavior. For example one way to define the normalization is to use Cramer's rule to solve (2) (see [11]). Then for the ASEP the normalization is given by $(\alpha\beta)^N$ times the expression (3) and additional zeros are introduced only at the origin.

Finally we remark on the applicability of the Lee-Yang theory to other nonequilibrium systems. Firstly, a generalization of the ASEP that allows particles also to hop to the left at a rate q has been solved [20]. The phase behavior when $q < 1$ is very similar to that of the ASEP, and the rate q enters into the expressions for the current in a simple way. The result of this would be for the pattern of zeros in the α-plane to shrink towards the origin as $q \to 1$. At this point, there is a transition to a regime where the current ceases to flow in the thermodynamic limit. It would be of interest to see whether the zeros of the normalization in the complex-q plane accumulate at $q = 1$ since this would provide some evidence for the generality of the Lee-Yang picture when applied to complex transition rates. Further evidence is provided by a study of the percolation probability on finite directed percolation lattices [21] in which a similar accumulation phenomenon to that reported here was observed. Also, one might learn something of the approach to the thermodynamic limit by considering how the distribution of zeros varies as the system size is increased.

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